Adiabatic expansion approximation solutions for the three-body problem

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Abstract

The motion of a muon in two centers coulomb field is one of the interesting problems of quantum mechanics. The adiabatic expansion method is powerful approach to study the muonic three-body system. In this investigation the three-body problem is studied for short-range interactions. Bound states and energy levels of this system were calculated and compared with their Born-Oppenheimer method counterparts. The obtained results are in good agreement with the previous calculations.

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1 Introduction

A negative muon is a lepton of the second generation with mass number about times heavier than that of electrons, and has a finite lifetime of $\tau_\mu = 2.197\mu sec$. Nuclear fusion reactions can be catalyzed in a suitable fusion fuel by muons [1-3]. Energetic negative Muons, after stopping in a hydrogen isotope $H_2/D_2/T_2$ mixture, fuse with different hydrogen isotopes to form the muonic atoms $p\mu$, $d\mu$ and $t\mu$ in excited states. The size of a muonic atom is about 209 times smaller than a normal atom. After a sequence of cascade transitions lasting about $10^{-11}sec$ at liquid hydrogen density ($L.H.D \approx 4.25 \times 10^{22} atoms/cm^3$), muonic atoms are formed in the ground $1S$-state with kinetic energy in the range of $10^{-3} - 10^2 eV$, depending on the temperature of the target and the prehistory of cascade transitions[4,5]. Muonic molecular formation may take place in collisions of the muonic atom in its ground state with ordinary hydrogen molecules.
The crucial process is the resonant formation of the muonic molecule $dt\mu$ into the loosely bound rotational-vibrational state $J = 1$, $\nu = 1$ ($10^{-8} - 10^{-10} sec$). This state quickly de-excites to $J = 0$ levels, from which the two nuclei fuse ($\approx 10^{-12}$). Usually the muon is free to start the next cycle,

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but occasionally (with probability $\omega_s \simeq 0.555\%$ in a D-T target at density $\phi = 1.2\ L.H.D$ [6]) it is removed from the active cycle by "sticking" to the helium nucleus. Resonant formation of the $dd\mu$ molecule at very low temperatures was observed in solid and liquid D_2 targets [7,8]. Energy levels of muonic molecules in muon catalyzed fusion (μCF) systems have been extensively studied with various calculational methods [9-12]. The solution of the non-relativistic Schrodinger equation for the three-body system was found using two different methods: by: the adiabatic expansion method and Born-Oppenheimer method. The Born-Oppenheimer approach assumes the nuclei to be infinitely heavy with respect to the negatively charged particle. It should be kept in mind that the following Born-Oppenheimer approach is the simplest solution to the three-body coulomb system. This approach is expected to be a poor approximation for calculations of muonic molecule eigenvalues. In the present paper, we calculate binding energies of the bound states of the $dd\mu$ muonic molecule using the adiabatic expansion method.

2 Theoretical calculations

The exact Hamiltonian that describes muonic three-body system can be shown by following relation:

$$H = -\frac{1}{2m_1}\nabla^2_{R_1} - \frac{1}{2m_2}\nabla^2_{R_2} - \frac{1}{2m_\mu}\nabla^2_{R_\mu} - \frac{z_1 z_\mu}{|\mathbf{r}_\mu - \mathbf{R}_1|} - \frac{z_2 z_\mu}{|\mathbf{r}_\mu - \mathbf{R}_2|} + \frac{z_1 z_2}{|\mathbf{R}_1 - \mathbf{R}_2|} \tag{1}$$

where 1 and 2 denote the two nuclei, their position is given by R_1 and R_2, and the muon coordinate is r_μ. The center of mass coordinate R_{CM} is given by

$$\mathbf{R}_{CM} = \frac{m_1\mathbf{R}_1 + m_2\mathbf{R}_2 + m_\mu\mathbf{r}_\mu}{m_1 + m_2 + m_\mu} \tag{2}$$

It is convenient to define Jacobi coordinate r and R as follow:

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_\mu - \frac{\mathbf{R}_1 + \mathbf{R}_2}{2} \\ \mathbf{R} &= \mathbf{R}_2 - \mathbf{R}_1 \end{aligned} \tag{3}$$

where R is the internuclear coordinate and r is the muon coordinate to midpoint between the two nuclei. In these coordinates (R, r), the Hamiltonian denoted by equation (1) is change to the following operator:

$$H = -\frac{1}{2M_T}\nabla^2_{R_{CM}} - \frac{1}{2M}\left(\nabla_R + \frac{\lambda}{2}\nabla_r\right)^2 - \frac{1}{2m}\nabla^2_r - \frac{z_1 z_\mu}{|\mathbf{r}_\mu - \mathbf{R}_1|} - \frac{z_2 z_\mu}{|\mathbf{r}_\mu - \mathbf{R}_2|} + \frac{z_1 z_2}{|\mathbf{R}_1 - \mathbf{R}_2|} \tag{4}$$

where

$$\begin{aligned} M_T &= m_1 + m_2 + m_\mu \\ \frac{1}{M} &= \frac{1}{m_1} + \frac{1}{m_2} \\ \frac{1}{m} &= \frac{1}{m_1 + m_2} + \frac{1}{m_\mu} \\ \lambda &= \frac{m_1 - m_2}{m_1 + m_2} \end{aligned} \tag{5}$$

After separation of variables, the non-relativistic Hamiltonian in units of $e = \hbar = m_\mu = 1$, can be given by

$$H(\hat{o}, R) = -\frac{1}{2M}\left(\nabla_R + \frac{\lambda}{2}\nabla_r\right)^2 - H_1 + \frac{z_1 z_2}{R} \tag{6}$$

where

$$H_1 = -\frac{1}{2m}\nabla_r^2 - \frac{z_1}{r_1} - \frac{z_2}{r_2} \tag{7}$$

where $\hat{o}$ represent the five dimensional variable. We use the set $\hat{o} = (\Theta, \Phi, \xi, \eta, \varphi)$ where (Θ, Φ, φ) define the Euler rotation specifying the body-fixed frame with its unit vectors to coincide with the principal axes of the inertia tensor of a three-body system. The hyperspheroidal coordinates ξ and η are easily expressed by the muon-nucleus distances r_1, r_2 and the internuclear distance R,

$$\begin{aligned} \xi &= \frac{r_1 + r_2}{R}, \quad (1 \leq \xi < \infty) \\ \eta &= \frac{r_1 - r_2}{R}, \quad (-1 \leq \eta \leq 1) \end{aligned} \tag{8}$$

The three-body Hamiltonian (6) commutes with the total angular momentum operator for the three particle system, $\mathbf{J}$, its projection on z-axis, $\mathbf{J}_z$, and the total parity operator, $\mathbf{P}(\mathbf{R} \longrightarrow \mathbf{-R}, \mathbf{r} \longrightarrow \mathbf{-r})$. Eigenfunctions of the Hamiltonian in the total angular momentum representation reads:

$$\Psi^p_{J,M}(\mathbf{R}, \mathbf{r}) = \sum_{m=-J}^{J} F_m^{Jp}(R, \xi, \eta) D^{Jp}_{Mm}(\Phi, \Theta, \varphi) \tag{9}$$

Adiabatic expansion of radial function, $F_m^{Jp}(R, \xi, \eta)$ is usually written in the form:

$$F_m^{Jp}(R, \xi, \eta) = \sum_{N=1}^{\infty}\sum_{l=0}^{N-1} \psi_{Nlm}(R; \xi, \eta)\chi^{Jp}_{Nlm}(R)R^{-1} + \sum_{l=0}^{\infty}\int_0^{\infty} dk \psi_{klm}(R; \xi, \eta)\chi^{Jp}_{klm}(R)R^{-1} \tag{10}$$

where $\chi_i^{Jp}(R)$ describe relative motion of the nuclei. Let us consider the Wigner function, $D^{Jp}_{Mm}(\Phi, \Theta, \varphi)$ which is the eigenstates of $\mathbf{J}^2$, $\mathbf{J}_z$ and $\mathbf{R}.\mathbf{J}/\mathrm{R}$ with the eigenvlues $J(J+1)$, M and m [13]. It can be transformed under the inversion as follow:

$$\mathbf{P}D^J_{Mm}(\Phi, \Theta, \varphi) = D^J_{Mm}(\Phi + \pi, \pi - \Theta, \pi - \varphi) = (-1)^{J-m} D^J_{M,-m}(\Phi, \Theta, \varphi) \tag{11}$$

If $m \neq 0$, the resultant Wigner functions would be different, and the angular functions consist both even and odd combinations. It is convenient to specify these combinations as follows:

$$D^{Jp}_{Mm}(\Phi, \Theta, \varphi) = \frac{\sqrt{2J+1}}{4\pi}\left[(-1)^m D^J_{Mm}(\Phi, \Theta, \varphi) + p(-1)^J D^J_{M,-m}(\Phi, \Theta, \varphi)\right] \tag{12}$$

$P = \pm(-1)^J$ is the eigenvalue of the parity operator:

$$\mathbf{P}D^{Jp}_{Mm} = pD^{Jp}_{Mm} \tag{13}$$

The functions presented in equation (12)(in bracket) are satisfy the following orthonormality condition:

$$\int_0^{\pi} sin\Theta d\Theta \int_0^{2\pi} d\Phi \int_0^{2\pi} d\varphi \left[D^{Jp}_{Mm}(\Phi, \Theta, \varphi)\right]^* D^{J'p'}_{M'm'}(\Phi, \Theta, \varphi) = \delta_{JJ'}\delta_{pp'}\delta_{MM'}\delta_{mm'} \tag{14}$$

If $m = 0$, both the Wigner functions in (11) are reduced to the ordinary spherical function $Y_{JM}(\Theta, \Phi)$ so that the dependence of φ disappears and the angular functions satisfying the conditions (13) and (14) are:

$$D^{Jp}_{M,m=0}(\Phi, \Theta, \varphi) = \frac{Y_{JM}(\Theta, \Phi)}{\sqrt{2\pi}} \tag{15}$$

In this case the parity is unambiguously specified by the quantum number J: $p = +(-1)^J$. So, our basis functions have the following structure:

$$\Psi^{Jp}_{Mjm}(R, \Theta, \Phi, \xi, \eta, \varphi) = D^{Jp}_{M,m}(\Phi, \Theta, \varphi)\psi_{jm}(\xi, \eta; R)\frac{\chi^{Jp}_{jm}(R)}{R} \tag{16}$$

The wave functions $\Psi^{Jp}_{Mjm}(R, \Theta, \Phi, \xi, \eta, \varphi)$ describing reactions $h\mu + h$, $h = (p, d, t)$ can be decomposed over the solutions $\psi_{jm}(\xi, \eta; R)$ of the Coulomb two-center problem. $\psi_{jm}(\xi, \eta; R)$ is the complete set of solutions of the Coulomb two-center problem, therefore

$$H_1\psi_i(\xi, \eta; R)F(\varphi) = E_i(R)\psi_i(\xi, \eta; R)F(\varphi) \tag{17}$$

describing the muon motion around fixed nuclei separated by a distance R. $E_i(R)$ is the energy of a muon in the state i as a function of R. Here we show how to separate the variables through the use of the ellipsoidal (or, prolate spheroidal) coordinates

$$\begin{aligned} x &= \frac{R}{2}\sqrt{(\xi^2 - 1)(1 - \eta^2)}cos\varphi \\ y &= \frac{R}{2}\sqrt{(\xi^2 - 1)(1 - \eta^2)}sin\varphi \\ z &= \frac{R}{2}\xi\eta \end{aligned} \tag{18}$$

Note that the coordinates ξ, η and φ are orthogonal, and we have the first fundamental form

$$ds^2 = dx^2 + dy^2 + dz^2 = h^2_\xi d\xi^2 + h^2_\eta d\eta^2 + h^2_\varphi d\varphi^2 \tag{19}$$

where

$$\begin{aligned} h^2_\xi &= \left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 + \left(\frac{\partial z}{\partial \xi}\right)^2 = \frac{R^2}{4}\left(\frac{1 - \eta^2}{\xi^2 - 1}\right) \\ h^2_\eta &= \left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2 + \left(\frac{\partial z}{\partial \eta}\right)^2 = \frac{R^2}{4}\left(\frac{\xi^2 - 1}{1 - \eta^2}\right) \\ h^2_\varphi &= \left(\frac{\partial x}{\partial \varphi}\right)^2 + \left(\frac{\partial y}{\partial \varphi}\right)^2 + \left(\frac{\partial z}{\partial \varphi}\right)^2 = \frac{R^2}{4}\left(\xi^2 - 1\right)\left(1 - \eta^2\right) \end{aligned} \tag{20}$$

Thus

$$\begin{aligned} \nabla^2 &= \frac{1}{h_\xi h_\eta h_\varphi}\left[\frac{\partial}{\partial \xi}\left(\frac{h_\eta h_\varphi}{h_\xi}\frac{\partial}{\partial \xi}\right) + \frac{\partial}{\partial \eta}\left(\frac{h_\xi h_\varphi}{h_\eta}\frac{\partial}{\partial \eta}\right) + \frac{\partial}{\partial \varphi}\left(\frac{h_\xi h_\eta}{h_\varphi}\frac{\partial}{\partial \varphi}\right)\right] \\ &= \frac{4}{R^2(\xi^2 - \eta^2)}\left\{\frac{\partial}{\partial \xi}\left[(\xi^2 - 1)\frac{\partial}{\partial \xi}\right] + \frac{\partial}{\partial \eta}\left[(1 - \eta^2)\frac{\partial}{\partial \eta}\right] + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)}\frac{\partial^2}{\partial \varphi^2}\right\} \end{aligned} \tag{21}$$

Note that through the coordinate transformation (18), we have

$$r_1 = \frac{R}{2}(\xi + \eta) \tag{22}$$
$$r_2 = \frac{R}{2}(\xi - \eta)$$

Writing the wavefunction as $\psi_i(\xi, \eta; R)F(\varphi) = G(\xi)H(\eta)F(\varphi)$ and changing the variable to spheroidal coordinates, equation (17) can be separated into following three one-dimensional equations:

$$\frac{d^2F(\varphi)}{d\varphi^2} + m^2F(\varphi) = 0 \tag{23}$$

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{dG(\xi)}{d\xi}\right] + \left(-A + \alpha q\xi - q^2\xi^2 - \frac{m^2}{\xi^2-1}\right)G(\xi) = 0 \tag{24}$$

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{dH(\eta)}{d\eta}\right] + \left(+A - \beta q\eta + q^2\eta^2 - \frac{m^2}{1-\eta^2}\right)H(\eta) = 0 \tag{25}$$

where

$$\alpha = \frac{R}{q}(z_1 + z_2) \tag{26}$$
$$\beta = \frac{R}{q}(z_1 - z_2)$$

Note that A and q are unknown parameters and should be obtained from (24) and (25) as eigenvalues of the coupled system. Once A and q are obtained, then E can be obtained from $q^2 = -R^2E/2$. By substitution of expression (16) into the Schrodinger equation with Hamiltonian (6) and after averaging over spherical angles (Θ, Φ) and the muon state, one obtains the radial equation

$$\frac{1}{2M}\frac{d^2}{dR^2}\chi_i^J(R) + \left[\varepsilon - V_{B-O}(R) - U_i(R) - \frac{J(J+1)}{2MR^2}\right]\chi_i^J(R) = 0 \tag{27}$$

where $\varepsilon = E - E_i(\infty)$ is the collision energy and E is the total energy of the system and $E_i(\infty)$ is the ground state energy of muonic atom. $V_{B-O}(R) = E - E(\infty) + \frac{z_1z_2}{R}$ is the potential corresponding to the Born-Oppenheimer (B-O) approximation and $U_i(R) = \langle i|\left(H - H_1 - \frac{z_1z_2}{R}\right)|i\rangle$ is the adiabatic correction. The adiabatic potential $V_{Ad}(R)$ is:

$$V_{Ad}(R) = V_{B-O}(R) + U_i(R) \tag{28}$$

Table 1: Binding energies (eV) of the states (J, ν) for the $(dd\mu)$ muonic molecule.

(J, ν)	Ad(This work)	Ref. [14]	Ref. [15]
$(0, 0)$	325.06	325.0735	325.070 540
$(0, 1)$	35.79	35.8436	35.844 227
$(1, 0)$	226.62	226.6815	226.679 792
$(1, 1)$	1.73	1.97475	1.974 985
$(2, 0)$	86.20	86.4936	—

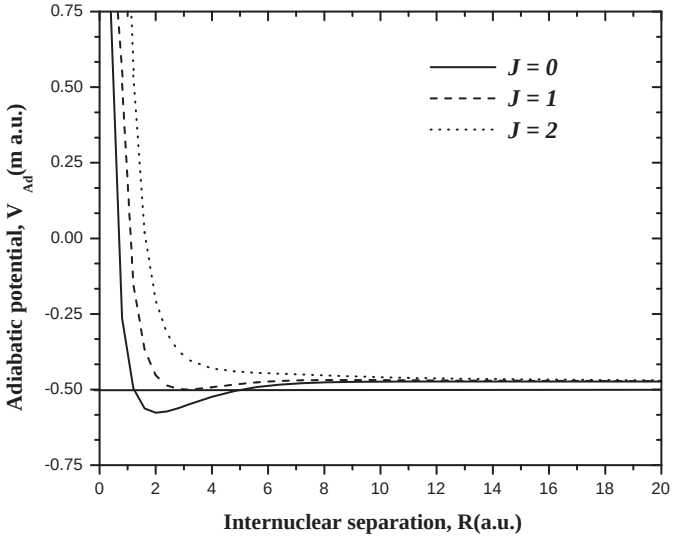

Figure 1: Adiabatic potential curves, V_{Ad}(J = 0, 1 and 2), corresponding to $d - d - \mu$ system.

The adiabatic potential $V_{Ad}(R)$ for the $(dd\mu)$ muonic molecule is calculated in the adiabatic expansion method. The adiabatic potential curves and qualitatively similar for each of muonic molecules and are displayed for $(dd\mu)$ in Figure 1. Results of the calculations of binding energies of the bound states (J, ν) of the $(dd\mu)$ muonic molecule are compared with the results of the other methods used in Refs. [14,15] and are given in Table 1.

3 conclusion

In this paper, we have presented the calculation of the binding energies of the symmetric muonic molecular ion. Early calculations were unable to demonstrate the existence of the crucial weakly bound states. For example, in the Born-Oppenheimer (fixed nuclei) approximation the state is

much too bound, but if adiabatic corrections are included it is not bound at all. The results are obtained by the three body Hamiltonian in the adiabatic expansion method. The calculated binding energies are in good agreement with the previous calculations by other authors using different methods.

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